Full wwPDB X-ray Structure Validation Report (i)

Nov 20, 2023 – 11:38 AM EST

PDB ID	:	1EWT
Title	:	CRYSTAL STRUCTURE OF METABOTROPIC GLUTAMATE RECEPTOR SUBTYPE 1 LIGAND FREE FORM I
Authors	:	Kunishima, N.; Shimada, Y.; Tsuji, Y.; Jingami, H.; Morikawa, K.
Deposited on	:	2000-04-27
Resolution	:	3.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

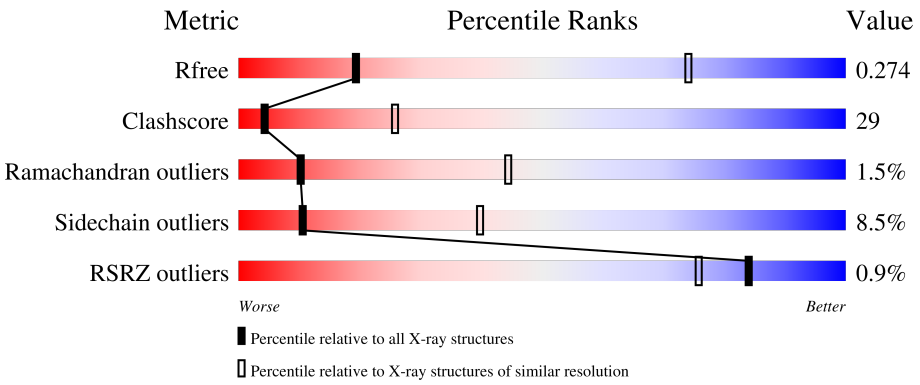
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	490	% 49% 41% • 7%
1	B	490	% 48% 39% 6% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	B	601	-	-	-	X

2 Entry composition (i)

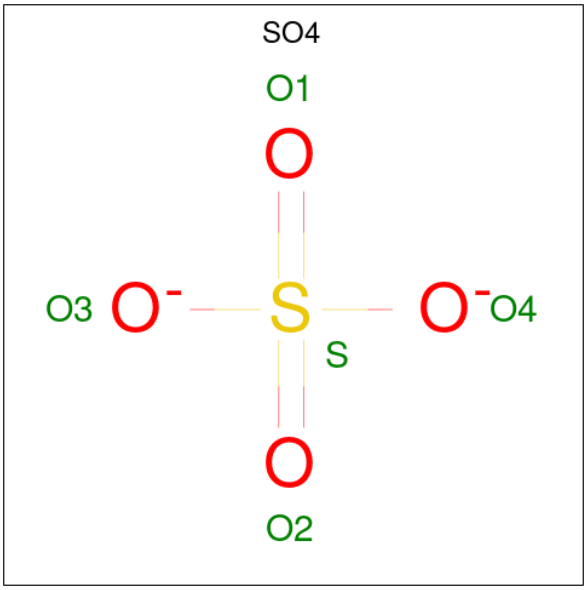
There are 3 unique types of molecules in this entry. The entry contains 7282 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called METABOTROPIC GLUTAMATE RECEPTOR SUBTYPE 1.

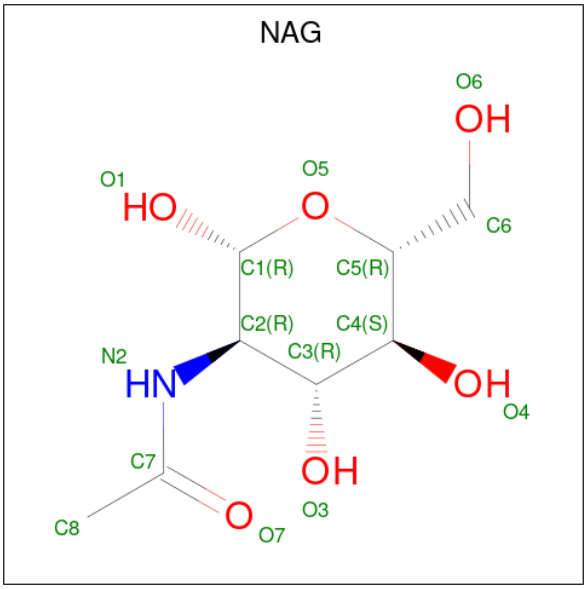
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	456	3624	2297	632	675	20	0	0	0
1	B	456	3624	2297	632	675	20	0	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	B	1	5	4	1	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



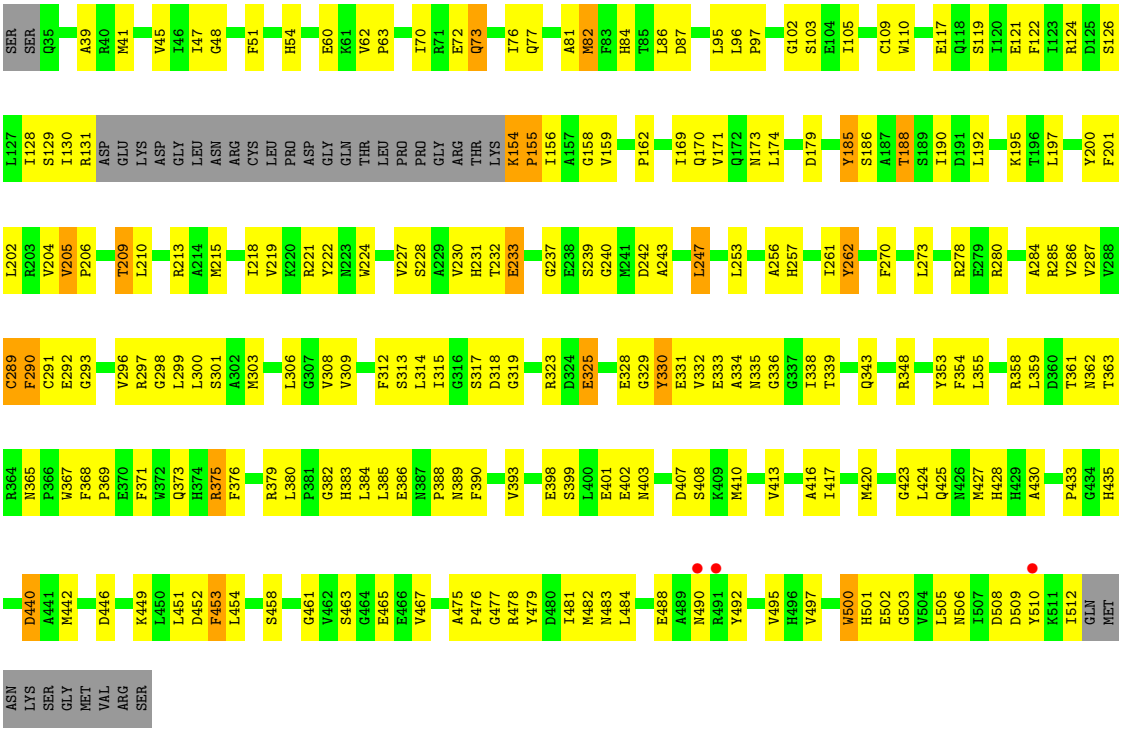
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	B	1	14	8	1	5	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

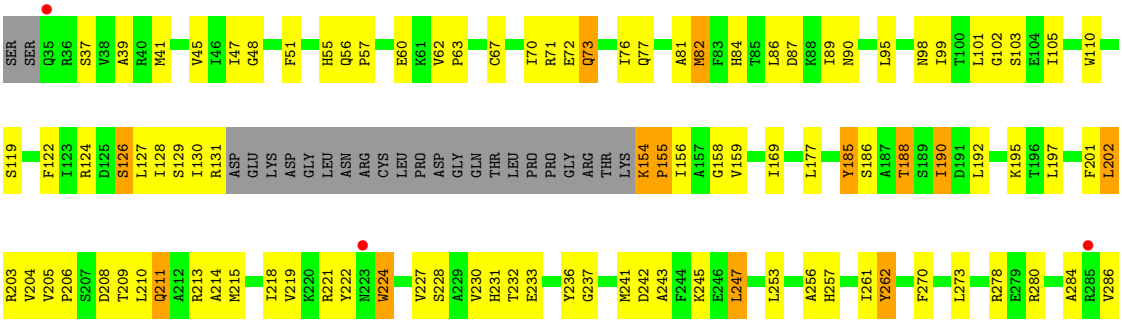
• Molecule 1: METABOTROPIC GLUTAMATE RECEPTOR SUBTYPE 1

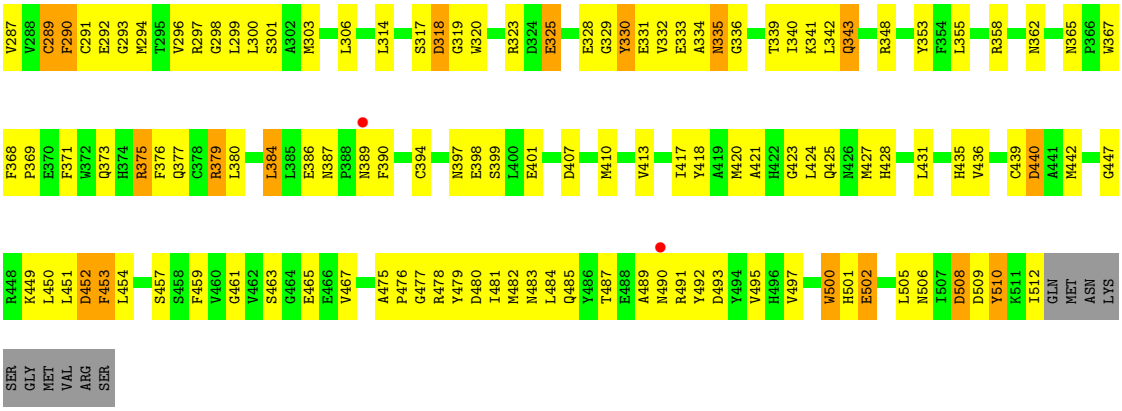
Chain A:



• Molecule 1: METABOTROPIC GLUTAMATE RECEPTOR SUBTYPE 1

Chain B:




V287 V288 C289 F290 C291 E292 G293 M294 T295 V296 R297 G298 L299 L300 S301 A302 M303 L306 L314 S317 D318 G319 W320 R323 D324 E325 E328 G329 Y330 E331 V332 E333 A334 N335 G336 T339 I340 K341 L342 Q343 R348 Y353 F354 L355 R358 N362 N365 P366 W367
F368 P369 E370 F371 W372 Q373 H374 R375 F376 Q377 C378 R379 L380 L384 L385 E386 N387 P388 N389 F390 C394 N397 E398 S399 L400 E401 D407 M410 V413 I417 Y418 A419 M420 A421 H422 G423 L424 Q425 N426 M427 H428 L431 H435 V436 C439 D440 A441 M442 G447
R448 K449 L450 L451 D452 F453 L454 S457 S458 F459 V460 G461 V462 S463 G464 E465 E466 V467 A475 P476 G477 R478 Y479 D480 I481 M482 N483 L484 Q485 Y486 T487 E488 A489 N490 R491 Y492 D493 Y494 V495 H496 V497 W500 H501 E502 L505 N506 I507 D508 D509 Y510 K511 I512 GLN MET ASN LYS
SER GLY MET VAL ARG SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	111.44Å 111.44Å 293.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 3.70 12.02 – 3.71	Depositor EDS
% Data completeness (in resolution range)	99.7 (12.00-3.70) 99.8 (12.02-3.71)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.32 (at 3.70Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.244 , 0.287 0.233 , 0.274	Depositor DCC
R_{free} test set	950 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	92.5	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 42.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7282	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.69	4/3704 (0.1%)	0.91	0/5009
1	B	0.68	4/3704 (0.1%)	0.90	0/5009
All	All	0.69	8/7408 (0.1%)	0.91	0/10018

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	224	TRP	NE1-CE2	8.77	1.49	1.37
1	B	500	TRP	NE1-CE2	8.74	1.49	1.37
1	A	500	TRP	NE1-CE2	8.70	1.48	1.37
1	A	224	TRP	NE1-CE2	8.68	1.48	1.37
1	A	110	TRP	NE1-CE2	8.59	1.48	1.37
1	A	367	TRP	NE1-CE2	8.56	1.48	1.37
1	B	110	TRP	NE1-CE2	8.55	1.48	1.37
1	B	367	TRP	NE1-CE2	7.15	1.46	1.37

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3624	0	3553	217	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3624	0	3552	212	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
3	B	14	0	13	1	0
All	All	7282	0	7118	419	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 29.

All (419) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:ASN:HD21	1:A:365:ASN:HB3	1.22	1.00
1:A:278:ARG:HH11	1:A:306:LEU:HD21	1.28	0.98
1:B:278:ARG:HH11	1:B:306:LEU:HD21	1.29	0.97
1:B:407:ASP:HB3	1:B:410:MET:HB2	1.45	0.96
1:A:323:ARG:HB3	1:A:325:GLU:HG2	1.50	0.93
1:A:407:ASP:HB3	1:A:410:MET:HB2	1.49	0.93
1:B:323:ARG:HB3	1:B:325:GLU:HG2	1.50	0.91
1:A:228:SER:HB2	1:A:287:VAL:HG22	1.54	0.89
1:A:218:ILE:HD11	1:A:481:ILE:HD12	1.51	0.89
1:B:218:ILE:HD11	1:B:481:ILE:HD12	1.56	0.88
1:B:228:SER:HB2	1:B:287:VAL:HG22	1.55	0.87
1:B:461:GLY:HA3	1:B:465:GLU:HG3	1.57	0.86
1:B:257:HIS:HB2	1:B:280:ARG:HG3	1.57	0.85
1:B:300:LEU:CD2	1:B:334:ALA:HB2	2.09	0.83
1:A:162:PRO:HG3	1:A:171:VAL:HG21	1.61	0.82
1:A:39:ALA:HB3	1:A:105:ILE:HB	1.60	0.81
1:B:39:ALA:HB3	1:B:105:ILE:HB	1.62	0.81
1:A:257:HIS:HB2	1:A:280:ARG:HG3	1.62	0.80
1:B:205:VAL:HG23	1:B:206:PRO:HD2	1.61	0.80
1:A:48:GLY:O	1:A:159:VAL:HA	1.83	0.78
1:A:362:ASN:ND2	1:A:365:ASN:HB3	1.99	0.77
1:B:340:ILE:HG23	1:B:479:TYR:HB3	1.63	0.77
1:A:278:ARG:NH1	1:A:306:LEU:HD21	2.00	0.77
1:B:278:ARG:NH1	1:B:306:LEU:HD21	2.00	0.77
1:B:355:LEU:HD22	1:B:401:GLU:HG2	1.66	0.76
1:A:427:MET:HE1	1:A:449:LYS:HB3	1.65	0.76
1:A:202:LEU:N	1:A:202:LEU:HD23	2.01	0.76
1:B:368:PHE:HB3	1:B:369:PRO:HD3	1.67	0.76
1:B:427:MET:CE	1:B:442:MET:HG2	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:475:ALA:HB1	1:B:476:PRO:HD2	1.68	0.75
1:A:300:LEU:CD2	1:A:334:ALA:HB2	2.17	0.75
1:A:382:GLY:O	1:A:386:GLU:HB2	1.86	0.75
1:A:368:PHE:HB3	1:A:369:PRO:HD3	1.68	0.74
1:B:478:ARG:HG3	1:B:478:ARG:HH11	1.52	0.74
1:B:202:LEU:HD23	1:B:202:LEU:N	2.02	0.73
1:B:323:ARG:HB3	1:B:325:GLU:CG	2.18	0.73
1:B:423:GLY:HA3	1:B:454:LEU:HD23	1.70	0.73
1:B:73:GLN:HA	1:B:77:GLN:HE21	1.53	0.73
1:A:73:GLN:HA	1:A:77:GLN:HE21	1.54	0.72
1:B:427:MET:HE1	1:B:442:MET:HG2	1.71	0.72
1:A:72:GLU:O	1:A:77:GLN:HG3	1.89	0.72
1:A:300:LEU:CD1	1:A:334:ALA:HB2	2.20	0.71
1:B:215:MET:O	1:B:219:VAL:HG23	1.91	0.71
1:A:334:ALA:O	1:A:484:LEU:HD23	1.91	0.71
1:B:358:ARG:HG2	1:B:358:ARG:HH11	1.56	0.71
1:B:205:VAL:CG2	1:B:206:PRO:HD2	2.21	0.70
1:A:230:VAL:O	1:A:289:CYS:HA	1.90	0.70
1:A:323:ARG:HB3	1:A:325:GLU:CG	2.21	0.70
1:B:89:ILE:HG21	1:B:101:LEU:HD12	1.72	0.70
1:B:300:LEU:HD22	1:B:334:ALA:HB2	1.74	0.70
1:A:227:VAL:HG12	1:A:286:VAL:HB	1.74	0.70
1:A:355:LEU:HD22	1:A:401:GLU:HG2	1.74	0.70
1:B:211:GLN:HA	1:B:479:TYR:CE1	2.28	0.69
1:A:383:HIS:CG	1:A:384:LEU:H	2.10	0.68
1:B:98:ASN:CG	3:B:601:NAG:C1	2.59	0.68
1:B:243:ALA:O	1:B:247:LEU:HB2	1.94	0.67
1:A:215:MET:O	1:A:219:VAL:HG23	1.95	0.67
1:B:213:ARG:HH11	1:B:247:LEU:HD21	1.59	0.66
1:A:243:ALA:O	1:A:247:LEU:HB2	1.95	0.66
1:A:461:GLY:HA3	1:A:465:GLU:HG3	1.76	0.66
1:A:335:ASN:OD1	1:A:336:GLY:N	2.29	0.66
1:A:446:ASP:HB3	1:A:449:LYS:HD2	1.77	0.66
1:B:227:VAL:HG12	1:B:286:VAL:HB	1.78	0.66
1:A:427:MET:HA	1:A:453:PHE:CZ	2.31	0.65
1:B:232:THR:HG21	1:B:292:GLU:OE2	1.97	0.65
1:B:278:ARG:HH11	1:B:306:LEU:CD2	2.07	0.65
1:A:461:GLY:N	1:A:465:GLU:O	2.28	0.65
1:A:169:ILE:HD11	1:A:192:LEU:HG	1.80	0.64
1:A:202:LEU:HD23	1:A:202:LEU:H	1.62	0.64
1:A:278:ARG:HH11	1:A:306:LEU:CD2	2.08	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:GLU:O	1:B:77:GLN:HG3	1.97	0.64
1:A:95:LEU:HD12	1:A:96:LEU:N	2.13	0.63
1:B:169:ILE:HD11	1:B:192:LEU:HG	1.80	0.63
1:B:202:LEU:HD23	1:B:202:LEU:H	1.62	0.63
1:B:228:SER:CB	1:B:287:VAL:HG22	2.28	0.63
1:A:154:LYS:HB2	1:A:154:LYS:NZ	2.12	0.63
1:B:297:ARG:HH12	1:B:328:GLU:HB3	1.62	0.63
1:A:402:GLU:O	1:A:403:ASN:HB2	1.99	0.63
1:B:231:HIS:HA	1:B:291:CYS:SG	2.38	0.63
1:A:205:VAL:HG13	1:A:206:PRO:HD2	1.80	0.63
1:A:475:ALA:HB1	1:A:476:PRO:HD2	1.79	0.63
1:A:195:LYS:NZ	1:A:201:PHE:O	2.33	0.62
1:A:297:ARG:HH12	1:A:328:GLU:HB3	1.63	0.62
1:B:154:LYS:HB2	1:B:154:LYS:NZ	2.14	0.62
1:B:343:GLN:HB2	1:B:478:ARG:O	1.99	0.62
1:A:383:HIS:ND1	1:A:384:LEU:N	2.37	0.62
1:B:300:LEU:HD21	1:B:334:ALA:HB2	1.81	0.62
1:A:232:THR:HG21	1:A:292:GLU:HB2	1.81	0.62
1:B:185:TYR:HD1	1:B:186:SER:N	1.98	0.61
1:B:477:GLY:O	1:B:478:ARG:HG2	1.99	0.61
1:B:48:GLY:O	1:B:159:VAL:HA	2.00	0.61
1:A:124:ARG:HG3	1:B:124:ARG:HH21	1.65	0.61
1:A:128:ILE:C	1:A:130:ILE:H	2.03	0.61
1:A:47:ILE:O	1:A:103:SER:HB2	2.01	0.61
1:B:47:ILE:O	1:B:103:SER:HB2	1.99	0.61
1:A:227:VAL:HG21	1:A:253:LEU:HD21	1.82	0.61
1:B:261:ILE:HD13	1:B:270:PHE:CE2	2.36	0.60
1:A:369:PRO:O	1:A:373:GLN:HG3	2.01	0.60
1:A:449:LYS:O	1:A:453:PHE:HB2	2.01	0.60
1:A:204:VAL:HG11	1:A:416:ALA:HA	1.84	0.60
1:A:232:THR:O	1:A:237:GLY:HA3	2.02	0.60
1:A:227:VAL:CG2	1:A:253:LEU:HD21	2.31	0.60
1:B:228:SER:OG	1:B:284:ALA:HB1	2.02	0.59
1:B:478:ARG:HH11	1:B:478:ARG:CG	2.15	0.59
1:B:510:TYR:CD1	1:B:510:TYR:C	2.76	0.59
1:B:425:GLN:O	1:B:428:HIS:HB3	2.03	0.59
1:B:190:ILE:HD12	1:B:208:ASP:HB2	1.85	0.59
1:B:185:TYR:CD2	1:B:413:VAL:HG22	2.38	0.58
1:A:73:GLN:H	1:A:73:GLN:NE2	2.02	0.58
1:A:293:GLY:HA3	1:A:323:ARG:NH1	2.19	0.58
1:A:130:ILE:C	1:A:131:ARG:HG3	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:GLU:OE1	1:B:325:GLU:N	2.36	0.57
1:A:185:TYR:CD2	1:A:413:VAL:HG22	2.39	0.57
1:A:231:HIS:HA	1:A:291:CYS:SG	2.44	0.57
1:B:211:GLN:HE21	1:B:317:SER:HB2	1.69	0.57
1:A:261:ILE:HD13	1:A:270:PHE:CE2	2.39	0.57
1:B:369:PRO:O	1:B:373:GLN:HG3	2.05	0.57
1:A:228:SER:CB	1:A:287:VAL:HG22	2.31	0.57
1:B:213:ARG:HH11	1:B:247:LEU:CD2	2.18	0.57
1:A:124:ARG:HG3	1:B:124:ARG:NH2	2.20	0.57
1:B:227:VAL:CG2	1:B:253:LEU:HD21	2.35	0.56
1:A:51:PHE:HE1	1:A:185:TYR:HE2	1.53	0.56
1:A:158:GLY:HA3	1:A:420:MET:CE	2.35	0.56
1:B:463:SER:C	1:B:465:GLU:H	2.08	0.56
1:B:73:GLN:H	1:B:73:GLN:NE2	2.03	0.56
1:A:228:SER:OG	1:A:284:ALA:HB1	2.06	0.56
1:B:130:ILE:C	1:B:131:ARG:HG3	2.26	0.56
1:B:380:LEU:HD23	1:B:394:CYS:HB2	1.87	0.56
1:A:301:SER:HA	1:A:330:TYR:CE2	2.40	0.56
1:A:174:LEU:HB2	1:B:177:LEU:CD1	2.36	0.56
1:A:423:GLY:HA3	1:A:454:LEU:HD23	1.86	0.56
1:A:446:ASP:CB	1:A:449:LYS:HD2	2.35	0.56
1:B:335:ASN:HA	1:B:484:LEU:HD23	1.88	0.56
1:A:300:LEU:HD22	1:A:334:ALA:HB2	1.87	0.55
1:B:323:ARG:CB	1:B:325:GLU:HG2	2.30	0.55
1:B:407:ASP:O	1:B:410:MET:HB3	2.06	0.55
1:B:86:LEU:O	1:B:90:ASN:ND2	2.40	0.55
1:B:335:ASN:HD21	1:B:485:GLN:HA	1.72	0.55
1:B:331:GLU:HB3	1:B:492:TYR:CD2	2.41	0.54
1:B:478:ARG:HG3	1:B:478:ARG:NH1	2.19	0.54
1:B:463:SER:O	1:B:465:GLU:N	2.40	0.54
1:A:379:ARG:O	1:A:393:VAL:HG13	2.08	0.54
1:A:325:GLU:N	1:A:325:GLU:OE1	2.40	0.53
1:A:379:ARG:HD3	1:A:390:PHE:O	2.08	0.53
1:B:373:GLN:OE1	1:B:379:ARG:HA	2.08	0.53
1:B:451:LEU:HG	1:B:452:ASP:N	2.23	0.53
1:A:446:ASP:HB3	1:A:449:LYS:HB2	1.91	0.53
1:B:270:PHE:CE1	1:B:298:GLY:HA3	2.43	0.53
1:B:495:VAL:O	1:B:497:VAL:HG13	2.09	0.53
1:B:201:PHE:C	1:B:201:PHE:CD2	2.82	0.53
1:A:174:LEU:HB2	1:B:177:LEU:HD13	1.90	0.53
1:A:427:MET:HG2	1:A:442:MET:CE	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:GLN:HA	1:B:77:GLN:NE2	2.22	0.53
1:B:261:ILE:HD13	1:B:270:PHE:CD2	2.43	0.53
1:B:317:SER:O	1:B:319:GLY:N	2.41	0.53
1:A:45:VAL:HG11	1:A:424:LEU:CD1	2.39	0.53
1:B:427:MET:HE2	1:B:442:MET:HG2	1.88	0.53
1:B:119:SER:HA	1:B:122:PHE:HD2	1.74	0.52
1:A:300:LEU:HD13	1:A:334:ALA:HB2	1.90	0.52
1:B:51:PHE:HE1	1:B:185:TYR:HE2	1.55	0.52
1:A:82:MET:HE2	1:A:86:LEU:HD11	1.92	0.52
1:B:335:ASN:C	1:B:335:ASN:ND2	2.62	0.52
1:B:368:PHE:HB3	1:B:369:PRO:CD	2.38	0.52
1:A:95:LEU:HD12	1:A:96:LEU:H	1.73	0.52
1:A:232:THR:HG21	1:A:292:GLU:OE2	2.09	0.52
1:A:339:THR:OG1	1:A:482:MET:HB2	2.09	0.52
1:B:230:VAL:O	1:B:289:CYS:HA	2.10	0.52
1:B:377:GLN:HA	1:B:390:PHE:CE2	2.44	0.52
1:A:368:PHE:HB3	1:A:369:PRO:CD	2.39	0.52
1:B:340:ILE:CG2	1:B:479:TYR:HB3	2.37	0.52
1:A:270:PHE:CE1	1:A:298:GLY:HA3	2.45	0.52
1:B:301:SER:HA	1:B:330:TYR:CE2	2.45	0.52
1:B:335:ASN:ND2	1:B:485:GLN:HA	2.25	0.52
1:A:185:TYR:C	1:A:185:TYR:HD1	2.14	0.52
1:A:124:ARG:CG	1:B:124:ARG:NH2	2.74	0.51
1:A:185:TYR:C	1:A:185:TYR:CD1	2.84	0.51
1:A:386:GLU:O	1:A:388:PRO:HD3	2.10	0.51
1:B:489:ALA:C	1:B:491:ARG:H	2.12	0.51
1:A:261:ILE:HD13	1:A:270:PHE:CD2	2.46	0.51
1:A:430:ALA:HB3	1:A:453:PHE:HZ	1.75	0.51
1:A:45:VAL:HG11	1:A:424:LEU:HD13	1.92	0.51
1:B:195:LYS:HE2	1:B:195:LYS:HA	1.92	0.51
1:B:293:GLY:HA3	1:B:323:ARG:NH1	2.25	0.51
1:A:210:LEU:O	1:A:213:ARG:HB3	2.10	0.51
1:A:329:GLY:C	1:A:331:GLU:H	2.14	0.51
1:A:383:HIS:CG	1:A:384:LEU:N	2.77	0.51
1:A:73:GLN:HA	1:A:77:GLN:NE2	2.24	0.50
1:A:373:GLN:NE2	1:A:385:LEU:O	2.44	0.50
1:B:398:GLU:OE1	1:B:398:GLU:N	2.42	0.50
1:B:57:PRO:HG3	1:B:67:CYS:HA	1.93	0.50
1:A:185:TYR:HD1	1:A:186:SER:N	2.09	0.50
1:A:317:SER:O	1:A:319:GLY:N	2.44	0.50
1:B:461:GLY:N	1:B:465:GLU:O	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:ARG:HG3	1:A:376:PHE:CE2	2.47	0.50
1:A:126:SER:O	1:A:130:ILE:HG12	2.12	0.50
1:B:505:LEU:HD12	1:B:506:ASN:N	2.26	0.50
1:A:190:ILE:HD11	1:A:239:SER:O	2.12	0.50
1:A:47:ILE:O	1:A:103:SER:HA	2.11	0.50
1:A:202:LEU:N	1:A:202:LEU:CD2	2.70	0.50
1:A:427:MET:CE	1:A:449:LYS:HB3	2.39	0.50
1:B:47:ILE:HG23	1:B:420:MET:HG2	1.94	0.50
1:B:233:GLU:HB3	1:B:262:TYR:CD2	2.47	0.49
1:A:77:GLN:O	1:A:81:ALA:N	2.43	0.49
1:A:158:GLY:HA3	1:A:420:MET:HE1	1.94	0.49
1:A:119:SER:HA	1:A:122:PHE:HD2	1.75	0.49
1:A:463:SER:O	1:A:465:GLU:N	2.45	0.49
1:A:73:GLN:H	1:A:73:GLN:HE21	1.59	0.49
1:A:483:ASN:OD1	1:A:512:ILE:HG23	2.11	0.49
1:B:227:VAL:HG21	1:B:253:LEU:HD21	1.95	0.49
1:A:124:ARG:HH21	1:B:124:ARG:HG3	1.76	0.49
1:B:77:GLN:O	1:B:81:ALA:N	2.38	0.49
1:A:505:LEU:HD12	1:A:506:ASN:N	2.28	0.49
1:A:84:HIS:O	1:A:87:ASP:HB2	2.13	0.49
1:B:62:VAL:HB	1:B:63:PRO:HD3	1.94	0.49
1:B:158:GLY:HA3	1:B:420:MET:CE	2.41	0.49
1:B:169:ILE:HD12	1:B:192:LEU:HD21	1.95	0.49
1:B:339:THR:OG1	1:B:482:MET:HB2	2.12	0.49
1:B:435:HIS:CD2	1:B:439:CYS:HB3	2.47	0.49
1:A:218:ILE:HD11	1:A:481:ILE:CD1	2.34	0.49
1:A:388:PRO:O	1:A:390:PHE:N	2.46	0.49
1:B:126:SER:O	1:B:130:ILE:HG12	2.13	0.49
1:B:45:VAL:HG11	1:B:424:LEU:CD1	2.43	0.49
1:B:122:PHE:CD1	1:B:156:ILE:HG13	2.47	0.49
1:A:306:LEU:HG	1:A:308:VAL:HG13	1.95	0.48
1:A:488:GLU:N	1:A:488:GLU:CD	2.67	0.48
1:B:99:ILE:HD11	1:B:428:HIS:CD2	2.48	0.48
1:B:427:MET:HG2	1:B:431:LEU:HD12	1.95	0.48
1:B:510:TYR:CD1	1:B:510:TYR:O	2.67	0.48
1:A:96:LEU:N	1:A:97:PRO:HD3	2.28	0.48
1:A:407:ASP:O	1:A:410:MET:HB3	2.13	0.48
1:A:62:VAL:HB	1:A:63:PRO:HD3	1.96	0.48
1:B:213:ARG:NH1	1:B:247:LEU:HD21	2.29	0.48
1:B:478:ARG:CG	1:B:478:ARG:NH1	2.68	0.48
1:A:375:ARG:HG3	1:A:376:PHE:CD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:MET:HE1	1:A:449:LYS:CB	2.40	0.48
1:B:45:VAL:HG11	1:B:424:LEU:HD13	1.96	0.48
1:B:158:GLY:HA3	1:B:420:MET:HE1	1.95	0.48
1:B:70:ILE:HD13	1:B:371:PHE:HB2	1.95	0.48
1:A:122:PHE:CD1	1:A:156:ILE:HG13	2.48	0.47
1:A:510:TYR:CD1	1:A:510:TYR:C	2.88	0.47
1:B:70:ILE:HD11	1:B:76:ILE:HD11	1.96	0.47
1:B:202:LEU:N	1:B:202:LEU:CD2	2.71	0.47
1:A:47:ILE:N	1:A:102:GLY:O	2.44	0.47
1:A:301:SER:HA	1:A:330:TYR:HE2	1.78	0.47
1:A:81:ALA:HB2	1:A:410:MET:HE1	1.95	0.47
1:A:47:ILE:HG23	1:A:420:MET:HG2	1.96	0.47
1:A:190:ILE:HD13	1:A:243:ALA:HB2	1.96	0.47
1:B:329:GLY:C	1:B:331:GLU:H	2.17	0.47
1:B:427:MET:CG	1:B:431:LEU:HD12	2.45	0.47
1:A:192:LEU:HD22	1:A:201:PHE:CD1	2.49	0.47
1:B:195:LYS:NZ	1:B:201:PHE:O	2.48	0.47
1:A:162:PRO:HG3	1:A:171:VAL:CG2	2.40	0.47
1:B:375:ARG:HG3	1:B:376:PHE:CE2	2.50	0.47
1:B:82:MET:CE	1:B:86:LEU:HD11	2.45	0.47
1:B:73:GLN:H	1:B:73:GLN:HE21	1.62	0.47
1:B:124:ARG:O	1:B:128:ILE:HG12	2.15	0.46
1:B:154:LYS:HB2	1:B:154:LYS:HZ2	1.79	0.46
1:A:121:GLU:OE2	1:A:124:ARG:NH2	2.47	0.46
1:A:70:ILE:HD13	1:A:371:PHE:HB2	1.97	0.46
1:A:128:ILE:O	1:A:130:ILE:N	2.45	0.46
1:A:232:THR:OG1	1:A:292:GLU:N	2.30	0.46
1:A:82:MET:CE	1:A:86:LEU:HD11	2.45	0.46
1:A:169:ILE:HD12	1:A:192:LEU:HD21	1.97	0.46
1:B:299:LEU:O	1:B:303:MET:HG3	2.16	0.46
1:B:380:LEU:CD2	1:B:394:CYS:HB2	2.45	0.46
1:A:427:MET:HA	1:A:453:PHE:CE2	2.51	0.46
1:B:190:ILE:HD11	1:B:209:THR:N	2.31	0.46
1:A:204:VAL:HG11	1:A:416:ALA:CA	2.44	0.46
1:A:500:TRP:CH2	1:A:503:GLY:N	2.83	0.46
1:B:227:VAL:HG22	1:B:253:LEU:HD21	1.97	0.46
1:B:362:ASN:HD21	1:B:365:ASN:HB3	1.81	0.46
1:B:192:LEU:HD22	1:B:201:PHE:CD1	2.51	0.46
1:B:211:GLN:NE2	1:B:317:SER:HB2	2.30	0.46
1:A:47:ILE:HD12	1:A:86:LEU:HD21	1.97	0.46
1:A:402:GLU:O	1:A:402:GLU:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:TYR:HB2	1:A:500:TRP:HB3	1.97	0.46
1:A:201:PHE:CD2	1:A:201:PHE:C	2.88	0.46
1:B:424:LEU:HD23	1:B:450:LEU:HD13	1.97	0.46
1:B:332:VAL:HG23	1:B:333:GLU:N	2.31	0.45
1:A:361:THR:O	1:A:363:THR:HG23	2.15	0.45
1:B:205:VAL:HG23	1:B:342:LEU:HD21	1.98	0.45
1:A:335:ASN:ND2	1:A:492:TYR:CE1	2.84	0.45
1:B:454:LEU:O	1:B:457:SER:HB2	2.15	0.45
1:A:154:LYS:HB2	1:A:154:LYS:HZ2	1.78	0.45
1:B:98:ASN:HB2	1:B:436:VAL:HG12	1.97	0.45
1:B:185:TYR:CE2	1:B:413:VAL:HG22	2.52	0.45
1:B:270:PHE:O	1:B:273:LEU:HB3	2.17	0.45
1:B:317:SER:C	1:B:319:GLY:H	2.20	0.45
1:A:188:THR:HG22	1:A:206:PRO:O	2.17	0.45
1:A:296:VAL:O	1:A:299:LEU:N	2.50	0.45
1:A:239:SER:OG	1:A:240:GLY:N	2.49	0.45
1:A:128:ILE:C	1:A:130:ILE:N	2.71	0.45
1:A:461:GLY:HA3	1:A:465:GLU:CG	2.45	0.45
1:B:508:ASP:OD1	1:B:510:TYR:CD2	2.70	0.45
1:A:458:SER:HA	1:A:467:VAL:O	2.16	0.45
1:A:495:VAL:O	1:A:497:VAL:HG13	2.16	0.45
1:B:84:HIS:O	1:B:87:ASP:HB2	2.16	0.45
1:A:70:ILE:HD11	1:A:76:ILE:HD11	1.99	0.44
1:A:343:GLN:HE21	1:A:343:GLN:HB2	1.47	0.44
1:B:301:SER:HA	1:B:330:TYR:HE2	1.82	0.44
1:B:332:VAL:HG23	1:B:333:GLU:H	1.82	0.44
1:B:483:ASN:OD1	1:B:512:ILE:HG23	2.17	0.44
1:A:317:SER:C	1:A:319:GLY:H	2.21	0.44
1:A:463:SER:C	1:A:465:GLU:H	2.21	0.44
1:A:82:MET:HA	1:A:417:ILE:CD1	2.47	0.44
1:A:425:GLN:O	1:A:428:HIS:HB3	2.16	0.44
1:A:501:HIS:C	1:A:502:GLU:HG2	2.38	0.44
1:B:190:ILE:CD1	1:B:208:ASP:HB2	2.46	0.44
1:A:130:ILE:HG22	1:A:130:ILE:O	2.17	0.44
1:A:343:GLN:NE2	1:A:478:ARG:HB3	2.31	0.44
1:A:205:VAL:HG13	1:A:206:PRO:CD	2.45	0.44
1:A:359:LEU:HD11	1:A:369:PRO:HA	2.00	0.44
1:A:124:ARG:O	1:A:128:ILE:HG12	2.17	0.44
1:A:204:VAL:CG1	1:A:416:ALA:HA	2.46	0.44
1:B:320:TRP:O	1:B:323:ARG:HG3	2.18	0.44
1:B:358:ARG:HH11	1:B:358:ARG:CG	2.28	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ILE:CG2	1:A:209:THR:H	2.30	0.43
1:A:287:VAL:HB	1:A:314:LEU:HD23	1.99	0.43
1:B:341:LYS:HG2	1:B:342:LEU:N	2.33	0.43
1:A:124:ARG:CG	1:B:124:ARG:HH21	2.31	0.43
1:A:490:ASN:O	1:A:490:ASN:CG	2.55	0.43
1:A:300:LEU:HD21	1:A:334:ALA:HB2	1.95	0.43
1:B:130:ILE:O	1:B:130:ILE:HG22	2.18	0.43
1:B:82:MET:HE2	1:B:86:LEU:HD11	2.01	0.43
1:B:211:GLN:NE2	1:B:318:ASP:OD1	2.49	0.43
1:B:236:TYR:CE2	1:B:290:PHE:CD2	3.06	0.43
1:A:195:LYS:HA	1:A:195:LYS:HE2	2.01	0.43
1:B:55:HIS:ND1	1:B:71:ARG:HD2	2.33	0.43
1:B:218:ILE:HD11	1:B:481:ILE:HG23	2.00	0.43
1:A:154:LYS:HG2	1:A:155:PRO:HD2	2.00	0.43
1:A:73:GLN:HE21	1:A:73:GLN:HB2	1.54	0.43
1:A:84:HIS:HB2	1:A:353:TYR:CE2	2.54	0.43
1:A:373:GLN:OE1	1:A:380:LEU:HG	2.18	0.43
1:B:82:MET:HA	1:B:417:ILE:CD1	2.49	0.43
1:B:449:LYS:O	1:B:453:PHE:HB2	2.19	0.43
1:A:54:HIS:O	1:A:109:CYS:HA	2.19	0.43
1:A:398:GLU:OE1	1:A:398:GLU:N	2.38	0.43
1:B:205:VAL:CG2	1:B:342:LEU:HD21	2.48	0.43
1:A:169:ILE:HG22	1:A:170:GLN:N	2.33	0.43
1:A:185:TYR:CE2	1:A:413:VAL:HG22	2.53	0.43
1:B:501:HIS:C	1:B:502:GLU:HG2	2.38	0.43
1:A:124:ARG:NH2	1:B:124:ARG:HG3	2.33	0.42
1:A:233:GLU:HB3	1:A:262:TYR:CE2	2.54	0.42
1:A:451:LEU:HG	1:A:452:ASP:N	2.33	0.42
1:B:380:LEU:O	1:B:386:GLU:HG3	2.19	0.42
1:A:47:ILE:O	1:A:103:SER:CB	2.66	0.42
1:A:221:ARG:C	1:A:222:TYR:HD2	2.22	0.42
1:A:285:ARG:HH11	1:A:285:ARG:HG3	1.83	0.42
1:B:221:ARG:HE	1:B:221:ARG:HB2	1.64	0.42
1:B:331:GLU:HG2	1:B:492:TYR:HB2	2.02	0.42
1:A:240:GLY:HA3	1:A:290:PHE:CE1	2.54	0.42
1:A:262:TYR:HD2	1:A:262:TYR:HA	1.74	0.42
1:B:47:ILE:HD12	1:B:86:LEU:HD21	2.01	0.42
1:B:122:PHE:HD1	1:B:156:ILE:HG13	1.84	0.42
1:B:185:TYR:O	1:B:205:VAL:HG11	2.19	0.42
1:B:221:ARG:C	1:B:222:TYR:HD2	2.22	0.42
1:A:270:PHE:O	1:A:273:LEU:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:LEU:HG	1:A:306:LEU:O	2.20	0.42
1:A:328:GLU:O	1:A:330:TYR:HD1	2.02	0.42
1:B:241:MET:HG3	1:B:245:LYS:HG3	2.00	0.42
1:A:358:ARG:NH1	1:A:358:ARG:HG2	2.34	0.42
1:B:47:ILE:N	1:B:102:GLY:O	2.49	0.42
1:B:185:TYR:CD1	1:B:186:SER:N	2.83	0.42
1:A:423:GLY:HA3	1:A:454:LEU:CD2	2.48	0.42
1:A:354:PHE:O	1:A:354:PHE:CG	2.72	0.42
1:B:84:HIS:HB2	1:B:353:TYR:CE2	2.55	0.42
1:B:477:GLY:C	1:B:478:ARG:HG2	2.40	0.42
1:A:173:ASN:HD22	1:A:173:ASN:HA	1.74	0.42
1:B:192:LEU:HD22	1:B:201:PHE:CG	2.54	0.42
1:B:358:ARG:HG2	1:B:358:ARG:NH1	2.30	0.42
1:A:308:VAL:O	1:A:309:VAL:CG2	2.68	0.42
1:A:119:SER:O	1:A:122:PHE:HB2	2.20	0.42
1:A:463:SER:C	1:A:465:GLU:N	2.73	0.41
1:B:328:GLU:O	1:B:330:TYR:HD1	2.02	0.41
1:A:124:ARG:NH2	1:B:124:ARG:CG	2.83	0.41
1:A:500:TRP:CZ3	1:A:502:GLU:HA	2.55	0.41
1:B:47:ILE:O	1:B:103:SER:HA	2.19	0.41
1:B:335:ASN:ND2	1:B:336:GLY:N	2.68	0.41
1:B:232:THR:O	1:B:237:GLY:HA3	2.20	0.41
1:B:343:GLN:HG3	1:B:480:ASP:CG	2.41	0.41
1:B:387:ASN:OD1	1:B:389:ASN:N	2.50	0.41
1:A:117:GLU:HG3	1:B:127:LEU:HD13	2.03	0.41
1:A:368:PHE:CB	1:A:369:PRO:HD3	2.45	0.41
1:A:407:ASP:CB	1:A:410:MET:HB2	2.35	0.41
1:B:287:VAL:HB	1:B:314:LEU:HD23	2.02	0.41
1:B:331:GLU:O	1:B:335:ASN:HB2	2.20	0.41
1:B:379:ARG:HB3	1:B:387:ASN:O	2.20	0.41
1:A:335:ASN:ND2	1:A:492:TYR:HE1	2.17	0.41
1:A:206:PRO:HB3	1:A:477:GLY:HA2	2.03	0.41
1:B:154:LYS:HG2	1:B:155:PRO:HD2	2.03	0.41
1:B:188:THR:HG22	1:B:206:PRO:O	2.20	0.41
1:B:296:VAL:O	1:B:299:LEU:N	2.52	0.41
1:B:459:PHE:CZ	1:B:467:VAL:HG11	2.55	0.41
1:A:84:HIS:HB2	1:A:353:TYR:CD2	2.56	0.41
1:B:214:ALA:HA	1:B:500:TRP:NE1	2.35	0.41
1:B:435:HIS:CD2	1:B:439:CYS:CB	3.04	0.41
1:A:169:ILE:CD1	1:A:192:LEU:HG	2.51	0.41
1:B:188:THR:HA	1:B:203:ARG:NH1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:GLN:HG3	1:B:480:ASP:OD2	2.21	0.41
1:B:384:LEU:H	1:B:384:LEU:HG	1.66	0.41
1:A:407:ASP:OD2	1:A:408:SER:N	2.54	0.41
1:B:208:ASP:O	1:B:211:GLN:HB2	2.20	0.41
1:B:169:ILE:CD1	1:B:192:LEU:HG	2.50	0.40
1:B:418:TYR:O	1:B:421:ALA:HB3	2.21	0.40
1:B:56:GLN:HA	1:B:57:PRO:HD3	1.95	0.40
1:A:179:ASP:HA	1:A:200:TYR:CE2	2.56	0.40
1:A:192:LEU:HD22	1:A:201:PHE:CG	2.56	0.40
1:A:315:ILE:HA	1:A:338:ILE:O	2.21	0.40
1:A:323:ARG:CB	1:A:325:GLU:HG2	2.35	0.40
1:B:222:TYR:N	1:B:222:TYR:CD2	2.87	0.40
1:B:222:TYR:HD1	1:B:224:TRP:CH2	2.38	0.40
1:B:236:TYR:CZ	1:B:290:PHE:HE2	2.40	0.40
1:B:317:SER:C	1:B:319:GLY:N	2.75	0.40
1:B:489:ALA:C	1:B:491:ARG:N	2.75	0.40
1:A:303:MET:CE	1:A:312:PHE:HD2	2.34	0.40
1:A:433:PRO:C	1:A:435:HIS:H	2.24	0.40
1:A:309:VAL:HG11	1:A:332:VAL:HG12	2.03	0.40
1:A:355:LEU:HD22	1:A:401:GLU:CG	2.49	0.40
1:B:236:TYR:CE2	1:B:290:PHE:CE2	3.10	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	452/490 (92%)	391 (86%)	55 (12%)	6 (1%)	12 47
1	B	452/490 (92%)	397 (88%)	47 (10%)	8 (2%)	8 41
All	All	904/980 (92%)	788 (87%)	102 (11%)	14 (2%)	10 44

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	256	ALA
1	A	389	ASN
1	B	256	ALA
1	A	318	ASP
1	A	330	TYR
1	A	440	ASP
1	B	318	ASP
1	B	440	ASP
1	B	508	ASP
1	A	129	SER
1	B	490	ASN
1	B	502	GLU
1	B	330	TYR
1	B	447	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	392/422 (93%)	365 (93%)	27 (7%)	15 46
1	B	392/422 (93%)	352 (90%)	40 (10%)	7 31
All	All	784/844 (93%)	717 (92%)	67 (8%)	10 40

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	MET
1	A	60	GLU
1	A	73	GLN
1	A	82	MET
1	A	154	LYS
1	A	155	PRO
1	A	185	TYR
1	A	188	THR
1	A	197	LEU

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Mol	Chain	Res	Type
1	A	205	VAL
1	A	209	THR
1	A	233	GLU
1	A	242	ASP
1	A	247	LEU
1	A	262	TYR
1	A	289	CYS
1	A	290	PHE
1	A	313	SER
1	A	325	GLU
1	A	333	GLU
1	A	348	ARG
1	A	375	ARG
1	A	399	SER
1	A	440	ASP
1	A	453	PHE
1	A	508	ASP
1	A	509	ASP
1	B	37	SER
1	B	41	MET
1	B	60	GLU
1	B	73	GLN
1	B	82	MET
1	B	95	LEU
1	B	126	SER
1	B	129	SER
1	B	154	LYS
1	B	155	PRO
1	B	185	TYR
1	B	188	THR
1	B	190	ILE
1	B	197	LEU
1	B	202	LEU
1	B	204	VAL
1	B	210	LEU
1	B	211	GLN
1	B	242	ASP
1	B	247	LEU
1	B	262	TYR
1	B	289	CYS
1	B	290	PHE
1	B	294	MET

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Mol	Chain	Res	Type
1	B	325	GLU
1	B	335	ASN
1	B	343	GLN
1	B	348	ARG
1	B	375	ARG
1	B	379	ARG
1	B	384	LEU
1	B	397	ASN
1	B	399	SER
1	B	440	ASP
1	B	452	ASP
1	B	453	PHE
1	B	487	THR
1	B	493	ASP
1	B	509	ASP
1	B	510	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	77	GLN
1	A	173	ASN
1	A	176	GLN
1	A	250	GLN
1	A	343	GLN
1	A	362	ASN
1	B	73	GLN
1	B	77	GLN
1	B	173	ASN
1	B	176	GLN
1	B	211	GLN
1	B	250	GLN
1	B	335	ASN
1	B	343	GLN
1	B	362	ASN
1	B	435	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	B	704	-	4,4,4	0.26	0	6,6,6	0.19	0
2	SO4	A	702	-	4,4,4	0.25	0	6,6,6	0.21	0
2	SO4	A	701	-	4,4,4	0.28	0	6,6,6	0.25	0
2	SO4	B	703	-	4,4,4	0.26	0	6,6,6	0.17	0
3	NAG	B	601	1	14,14,15	0.87	0	17,19,21	0.83	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	601	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	601	NAG	O5-C5-C6-O6
3	B	601	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	456/490 (93%)	-0.45	3 (0%)	87	81	32, 69, 110, 123	0
1	B	456/490 (93%)	-0.45	5 (1%)	80	71	31, 68, 112, 124	0
All	All	912/980 (93%)	-0.45	8 (0%)	84	76	31, 69, 112, 124	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	490	ASN	3.3
1	A	490	ASN	3.1
1	B	223	ASN	2.7
1	B	35	GLN	2.4
1	B	389	ASN	2.2
1	A	510	TYR	2.2
1	A	491	ARG	2.1
1	B	285	ARG	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	B	601	14/15	0.73	0.41	93,96,100,101	0
2	SO4	B	704	5/5	0.89	0.22	92,92,93,93	0
2	SO4	A	701	5/5	0.92	0.18	81,82,83,83	0
2	SO4	B	703	5/5	0.93	0.20	88,89,89,90	0
2	SO4	A	702	5/5	0.98	0.17	72,73,74,74	0

6.5 Other polymers (i)

There are no such residues in this entry.